Green functions and self-energy functionals

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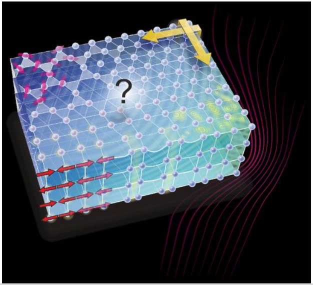

Prelude

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- We consider a Grand canonical ensemble at inverse temperature $\beta = 1/k_B T$ and chemical potential μ
- We introduce a complete set of single particle states $\phi_\alpha(x)$ - where for example $\alpha = (n, \mathbf{k}, \sigma), (i, \sigma)$ - and the corresponding Fermion operators $c^\dagger_\alpha$ and c_α
- The 'Grand canonical Hamiltonian' $K = H - \mu N$ is $K = K_0 + K_1$ with

$$K_0 = \sum_{\alpha,\beta} \left(t_{\alpha,\beta} - \mu\, \delta_{\alpha,\beta} \right) c^\dagger_\alpha c_\beta,$$

$$K_1 = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\; c^\dagger_\alpha c^\dagger_\beta c_\gamma c_\delta.$$

- Then (with $K\,|i\rangle = K_i\,|i\rangle$)

$$Z = \sum_i e^{-\beta K_i} \qquad \Omega = -\frac{1}{\beta} \log(Z) \qquad \langle O \rangle_{th} = \frac{1}{Z} \sum_i \langle i|O|i\rangle\, e^{-\beta K_i}$$

Green's function

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A Green's function describes the following *gedanken experiment*

$$\sum_i \langle i| e^{\frac{iKt'}{\hbar}} \; c_\beta^\dagger \; e^{\frac{-iK(t'-t)}{\hbar}} \; c_\alpha \; e^{\frac{-iKt}{\hbar}} \; |i\rangle \, \frac{e^{-\beta K_i}}{Z}$$

- Prepare the system in thermal equlibrium
- At time t remove a particle from state $\phi_\alpha(x)$
- Let the system evolve $t \to t'$ and reinsert a particle into state $\phi_\beta(x)$
- Determine overlap with undisturbed state

$$\Rightarrow \langle \, e^{\frac{iKt'}{\hbar}} c_\beta^\dagger e^{-\frac{iKt'}{\hbar}} \; e^{\frac{iKt}{\hbar}} c_\alpha e^{-\frac{iKt}{\hbar}} \, \rangle_{th} = \langle \, c_\beta^\dagger(t') \; c_\alpha(t) \, \rangle_{th}$$

Green's function

Define the imaginary time Heisenberg operators $(it \to \tau)$

$$c_\alpha(\tau) = e^{\frac{\tau K}{\hbar}}\ c_\alpha\ e^{-\frac{\tau K}{\hbar}} \qquad\qquad c^\dagger_\beta(\tau') = e^{\frac{\tau' K}{\hbar}}\ c^\dagger_\beta\ e^{-\frac{\tau' K}{\hbar}}$$

and

$$\begin{aligned}
G_{\alpha,\beta}(\tau,\tau') &= -\langle T\ c_\alpha(\tau)\ c^\dagger_\beta(\tau')\ \rangle_{th} \\
&= -\Theta(\tau-\tau')\langle\ c_\alpha(\tau)\ c^\dagger_\beta(\tau')\ \rangle_{th} + \Theta(\tau'-\tau)\langle\ c^\dagger_\beta(\tau')\ c_\alpha(\tau)\ \rangle_{th} \\
&= \frac{1}{Z}\Bigg(-\Theta(\tau-\tau')\sum_{i,j} e^{-\beta K_i}\ e^{\frac{\tau-\tau'}{\hbar}(K_i-K_j)}\ \langle i|c_\alpha|j\rangle\ \langle j|c^\dagger_\beta|i\rangle \\
&\qquad + \Theta(\tau'-\tau)\sum_{i,j} e^{-\beta K_i}\ e^{\frac{\tau-\tau'}{\hbar}(K_j-K_i)}\ \langle i|c^\dagger_\beta|j\rangle\ \langle j|c_\alpha|i\rangle\Bigg).
\end{aligned}$$

Only a function of $\tau - \tau'$

Fourier transform

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$$G_{\alpha,\beta}(\tau) = \frac{1}{Z}\Bigg(-\Theta(\tau) \sum_{i,j} e^{-\beta K_i}\, e^{\frac{\tau}{\hbar}(K_i-K_j)}\, \langle i|c_\alpha|j\rangle\, \langle j|c_\beta^\dagger|i\rangle$$

$$+\, \Theta(-\tau) \sum_{i,j} e^{-\beta K_i}\, e^{\frac{\tau}{\hbar}(K_j-K_i)}\, \langle i|c_\beta^\dagger|j\rangle\, \langle j|c_\alpha|i\rangle \Bigg)$$

- Well defined only for $\tau \in [-\beta\hbar, \beta\hbar] \Rightarrow$ Fourier frequencies $\frac{n\pi}{\hbar\beta}$
- $\tau \in [-\beta\hbar, 0] \Rightarrow G(\tau + \beta\hbar) = -G(\tau) \Rightarrow$ only odd n

$$G(\tau) = \frac{1}{\beta\hbar} \sum_{\nu=-\infty}^{\infty} e^{-i\omega_\nu \tau}\, G(i\omega_\nu) \qquad G(i\omega_\nu) = \int_0^{\beta\hbar} d\tau\, e^{i\omega_\nu \tau}\, G(\tau)$$

With the (Fermionic) Matsubara frequencies $\omega_\nu = \frac{(2\nu+1)\pi}{\beta\hbar}$

Equation of motion and self-energy

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We recall ...

$$G_{\alpha,\beta}(\tau) = -\langle T\, c_\alpha(\tau) c_\beta^\dagger(\tau') \,\rangle_{th}$$

$$= -\Theta(\tau)\langle\, c_\alpha(\tau)\; c_\beta^\dagger \,\rangle_{th} + \Theta(-\tau)\langle\, c_\beta^\dagger\; c_\alpha(\tau) \,\rangle_{th}$$

... and want to calculate $-\hbar\partial_\tau\, G_{\alpha,\beta}(\tau)$

We use $\partial_\tau\Theta(\pm\tau) = \pm\delta(\tau)$ and $-\hbar\partial_\tau c_\alpha^\dagger(\tau) = [c_\alpha^\dagger(\tau), K]$

$$-\hbar\partial_\tau G_{\alpha,\beta}(\tau) = \hbar\delta(\tau)\langle\, c_\alpha(\tau)\; c_\beta^\dagger + c_\beta^\dagger\; c_\alpha(\tau)\rangle_{th}$$

$$-\Theta(\tau)\langle\, [c_\alpha, K](\tau)\; c_\beta^\dagger \,\rangle_{th} + \Theta(-\tau)\langle\, c_\beta^\dagger\; [c_\alpha, K](\tau) \,\rangle_{th}$$

$$= \hbar\,\delta(\tau)\;\delta_{\alpha,\beta} - \langle T[c_\alpha, K](\tau)\; c_\beta^\dagger\rangle_{th}$$

Equation of motion and self-energy

We recall ...

$$-\hbar\partial_\tau G_{\alpha,\beta}(\tau) \quad = \quad \hbar\,\delta(\tau)\,\delta_{\alpha,\beta} - \langle T[c_\alpha, K](\tau)\; c^\dagger_\beta\rangle_{th}$$

... use ...

$$[c_\alpha, K] \quad = \quad \sum_\nu (t_{\alpha,\nu} - \mu\delta_{\alpha,\nu})\; c_\nu + \sum_{\nu,\lambda,\kappa} V_{\alpha,\nu,\kappa,\lambda}\; c^\dagger_\nu c_\lambda c_\kappa$$

... and find

$$-\hbar\partial_\tau G_{\alpha,\beta}(\tau) \quad = \quad \hbar\,\delta(\tau)\,\delta_{\alpha,\beta} + \sum_\nu (t_{\alpha,\nu} - \mu\delta_{\alpha,\nu})\; G_{\nu,\beta}(\tau) + F_{\alpha,\beta}(\tau)$$

$$F_{\alpha,\beta}(\tau) \quad = \quad -\sum_{\nu,\kappa,\lambda} V_{\alpha,\nu,\kappa,\lambda}\langle T[(c^\dagger_\nu c_\lambda c_\kappa)(\tau)\; c^\dagger_\beta]\rangle_{th}$$

Notice: $V_{\alpha,\nu,\kappa,\lambda} = 0$ (noninteracting system!) means $F = 0$

Equation of motion and self-energy

Recall

$$-\hbar\partial_\tau G_{\alpha,\beta}(\tau) \quad = \quad \hbar\,\delta(\tau)\,\delta_{\alpha,\beta} + \sum_\nu (t_{\alpha,\nu} - \mu\delta_{\alpha,\nu})\; G_{\nu,\beta}(\tau) + F_{\alpha,\beta}(\tau)$$

Fourier transformation gives

$$\left(i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar} \right) \mathbf{G}(i\omega_\nu) - \frac{1}{\hbar}\,\mathbf{F}(i\omega_\nu) \quad = \quad 1$$

Now define the self-energy $\mathbf{F}(i\omega_\nu) = \hbar\,\Sigma(i\omega_\nu)\;\mathbf{G}(i\omega_\nu)$ whence

$$\left(i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar} - \Sigma(i\omega_\nu) \right) \mathbf{G}(i\omega_\nu) \quad = \quad 1$$

In this way we arrive at the Dyson equation

$$\mathbf{G}^{-1}(i\omega_\nu) \quad = \quad i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar} - \Sigma(i\omega_\nu) = \mathbf{G}_0^{-1}(i\omega_\nu) - \Sigma(i\omega_\nu)$$

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Recall

$$\mathbf{G}_0^{-1}(i\omega_\nu) \quad = \quad i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}$$

For example $\alpha = (n, \mathbf{k}, \sigma)$,

$$H_0 \quad = \quad \sum_{n,\mathbf{k},\sigma} E_{n,\mathbf{k}}\; c^\dagger_{n,\mathbf{k},\sigma}\; c^\dagger_{n,\mathbf{k},\sigma}$$

$$\mathbf{G}_0^{-1}(i\omega_\nu) \quad = \quad i\omega_\nu - \frac{E_{n,\mathbf{k}}-\mu}{\hbar}$$

$$\mathbf{G}_0(i\omega_\nu) \quad = \quad \frac{1}{i\omega_\nu - \frac{E_{n,\mathbf{k}}-\mu}{\hbar}}$$

Summary so far

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- We have defined the Green's function which describes the *gedanken* experiment of adding/removing a particle at some time and undoing this at a different time
- It is related to the photoemission/inverse photoemission spectrum of the system and thus of considerable experimental relevance
- The Green's function of a noninteracting system is obtained from its equation of motion
- The effect of interactions can be concisely expressed in terms of the self-energy which gives the correction to the (inverse) noninteracting Green's function
- We proceed to give a representation of the Green's function in terms of a functional integral over Grassmann variables
- The derivation - which is not difficult but too lengthy to give here - can be found in the excellent textbook by Negele/Orland

Crash course in Grassmann variables

Grassmann variables are objects - here we write them as ϕ_i or ϕ_j^*, where i and j distinguish different Grassman variables - which anticommute

$$\phi_i^* \phi_j^* = -\phi_j^* \phi_i^* \qquad \phi_i \phi_j^* = -\phi_j^* \phi_i, \qquad \phi_i \phi_j = -\phi_j \phi_i.$$

- The asterisk * is part of the name of the Grassmann variable
- $\phi_i^* \phi_i^* = -\phi_i^* \phi_i^* = 0$ - The square of any Grassmann variable is zero
- A Grassmann algebra consists of all combinations of nonvanishing products of the 'Grassmann basis', e.g. with basis ϕ and ϕ^*

$$a_0 + a_1 \phi + a_2 \phi^* + a_3 \phi \phi^*$$

- The key property of Grassmann variables is the rule for 'integration'

$$\int d\phi \, \phi = 1, \qquad \int d\phi \, 1 = 0$$

Crash course in Grassmann variables

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- Functions of Grassmann variables are defined via the power series expansion

$$
\begin{aligned}
exp(a_1\phi + a_2\phi^* + a_3\phi^*\phi) &= 1 + (a_1\phi + a_2\phi^* + a_3\phi^*\phi) + \frac{1}{2!}a_1 a_2(\phi\phi^* + \phi^*\phi) \\
&= 1 + (a_1\phi + a_2\phi^* + a_3\phi^*\phi)
\end{aligned}
$$

Then we have

$$
\begin{aligned}
\int d\phi^*\, d\phi\, exp(a_1\phi + a_2\phi^* + a_3\phi^*\phi) &= a_3 \int d\phi^*\, d\phi\, \phi^*\, \phi \\
&= -a_3 \int d\phi^*\, d\phi\, \phi\, \phi^* \\
&= -a_3 \int d\phi^*\, \phi^* = -a_3
\end{aligned}
$$

Grassmann variable representation of Z

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- Let $[0, \hbar\beta]$ be divided into M intervals of length $\epsilon = \hbar\beta/M$
- Define imaginary time grid points $\tau_k = k \cdot \epsilon$, $k = 1 \ldots M$
- For each grid point τ_k introduce Grassmann variables $\phi^*_{\alpha,k}$ and $\phi_{\alpha,k}$
- α is the 'compound index' on Fermion operators $c^\dagger_\alpha$ and c_α
- Then $Z = \lim_{M\to\infty} Z_M$ whereby

$$Z_M = \prod_{k=1}^{M} \prod_{\alpha} \int d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}\, e^{-S(\phi^*,\phi)}$$

$$S(\phi^*,\phi) = \epsilon \sum_{k=1}^{M} \left[\sum_{\alpha} \phi^*_{\alpha,k} \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} + \frac{1}{\hbar} K(\phi^*_k, \phi_{k-1}) \right]$$

- $K(\phi^*_k, \phi_{k-1})$: Grand canonical Hamiltonian with $c^\dagger_\alpha \to \phi^*_{\alpha,k}$ and $c_\alpha \to \phi_{\alpha,k-1}$
- Important: $\phi_{\alpha,0} = -\phi_{\alpha,M}$

Grassman variable representation of Z

Recall

$$S(\phi^*,\phi) \quad = \quad \epsilon \sum_{k=1}^{M} \left[\sum_{\alpha} \phi^*_{\alpha,k} \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} + \frac{1}{\hbar} K(\phi^*_k, \phi_{k-1}) \right]$$

If we treat the Grassmann variables as ‘numbers’ and *nominally* let

$M \to \infty \Rightarrow \epsilon = \hbar\beta/M \to 0$

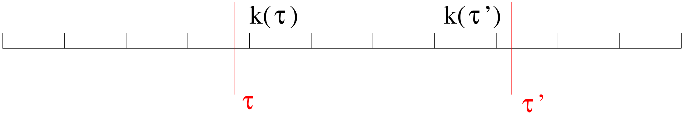
$$\Rightarrow S \quad \to \quad \int_0^{\hbar\beta} d\tau \left(\sum_{\alpha} \phi^*_{\alpha} \frac{\partial \phi_{\alpha}}{\partial \tau} + \frac{1}{\hbar} K(\phi^*, \phi) \right)$$

The Green's function

- Same imaginary-time grid as before

$$G_{\alpha,\beta}(\tau,\tau') \quad = \quad -\lim_{M\to\infty} \frac{\prod_{k=1}^{M} \prod_{\gamma} \int \, d\phi^{*}_{\gamma,k} \, d\phi_{\gamma,k} \, \phi_{\alpha,k(\tau)} \phi^{*}{}_{\beta,k(\tau')} \; e^{-S(\phi^{*},\phi)}}{\prod_{k=1}^{M} \prod_{\gamma} \int \, d\phi^{*}_{\gamma,k} \, d\phi_{\gamma,k} \; e^{-S(\phi^{*},\phi)}}$$

- $k(\tau)$ and $k(\tau')$: points on imaginary-time grid closest to τ and τ'



Fourier transform of S

Recall: $\phi_{\gamma,0} = -\phi_{\gamma,M}$ - to incorporate this define

$$\tilde{\phi}^*_{\gamma,\nu} = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} e^{-i\,\omega_\nu \tau_k}\,\phi^*_{\gamma,k}, \qquad \tilde{\phi}_{\gamma,\nu} = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} e^{i\,\omega_\nu \tau_k}\,\phi_{\gamma,k}$$

with $\omega_\nu = \frac{(2\nu+1)\pi}{\hbar\beta}$ (Fermionic Matsubara frequencies!) - this can be reverted

$$\phi^*_{\gamma,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{i\omega_\nu\,\tau_k}\tilde{\phi}^*_{\gamma,\nu}, \qquad \phi_{\gamma,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{-i\omega_\nu\,\tau_k}\tilde{\phi}_{\gamma,\nu}.$$

- The transformation $\phi^*_{\gamma,k} \to \tilde{\phi}^*_{\gamma,\nu}$ is unitary $\Rightarrow$ the Jacobian is unity
- The limit $M \to \infty$ is trivial to take

Fourier transform of S: K_0

$$K_0 = (t_{\alpha,\beta} - \mu\, \delta_{\alpha,\beta})\; c^\dagger_\alpha c_\beta \quad \Rightarrow \quad \epsilon \sum_{k=1}^{M} \left(t_{\alpha,\beta} - \mu \delta_{\alpha,\beta}\right) \phi^*_{\alpha,k}\, \phi_{\beta,k-1}$$

Insert the Fourier amplitudes

$$\phi^*_{\alpha,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{i\omega_\nu\, \tau_k}\; \tilde{\phi}^*_{\alpha,\nu} \qquad \phi_{\beta,k-1} = \frac{1}{\sqrt{M}} \sum_{\nu'=-\frac{M}{2}+1}^{\frac{M}{2}} e^{-i\omega_{\nu'}\,(\tau_k - \epsilon)}\; \tilde{\phi}_{\beta,\nu'}$$

$$\epsilon \sum_{k=1}^{M} \left(t_{\alpha,\beta} - \mu \delta_{\alpha,\beta}\right) \phi^*_{\alpha,k}\, \phi_{\beta,k-1} =$$

$$= \sum_{\nu,\nu'} \frac{\epsilon}{M} \sum_{k=1}^{M} e^{i(\omega_\nu - \omega_{\nu'})\tau_k}\; e^{i\omega_{\nu'}\epsilon} \left(t_{\alpha,\beta} - \mu \delta_{\alpha,\beta}\right)\; \tilde{\phi}^*_{\alpha,\nu}\; \tilde{\phi}_{\beta,\nu'}$$

$$= \epsilon \sum_{\nu} e^{i\omega_\nu \epsilon} \left(t_{\alpha,\beta} - \mu \delta_{\alpha,\beta}\right) \tilde{\phi}^*_{\alpha,\nu}\; \tilde{\phi}_{\beta,\nu}$$

Fourier transform of S: derivative term

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$$\phi^*_{\alpha,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{i\omega_\nu \tau_k} \tilde{\phi}^*_{\alpha,\nu} \qquad \phi_{\beta,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{-i\omega_\nu \tau_k} \tilde{\phi}_{\beta,\nu}$$

$$\begin{aligned}
\epsilon \sum_{k=1}^{M} \phi^*_{\alpha,k} \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} &= \sum_{\nu,\nu'} \frac{\epsilon}{M} \sum_{k=1}^{M} e^{i(\omega_\nu - \omega_{\nu'})\tau_k} \left[\frac{1 - e^{i\omega_{\nu'}\epsilon}}{\epsilon} \right] \tilde{\phi}^*_{\alpha,\nu} \tilde{\phi}_{\alpha,\nu'} \\
&= \epsilon \sum_{\nu} \left[\frac{1 - e^{i\omega_\nu \epsilon}}{\epsilon} \right] \tilde{\phi}^*_{\alpha,\nu} \tilde{\phi}_{\alpha,\nu} \\
&= \epsilon \sum_{\nu} e^{i\omega_\nu \epsilon} \left[\frac{e^{-i\omega_\nu \epsilon} - 1}{\epsilon} \right] \tilde{\phi}^*_{\alpha,\nu} \tilde{\phi}_{\alpha,\nu} \\
&\to \epsilon \sum_{\nu} e^{i\omega_\nu \epsilon} \quad (-i\omega_\nu) \quad \tilde{\phi}^*_{\alpha,\nu} \tilde{\phi}_{\alpha,\nu}
\end{aligned}$$

Fourier transform of S

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Combining the results we find that

$$S_0[\phi^*, \phi] = \epsilon \sum_{k=1}^{M} \left[\sum_{\alpha} \phi^*_{\alpha,k} \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} + \frac{1}{\hbar} K_0(\phi^*_k, \phi_{k-1}) \right]$$

$$= \epsilon \sum_{\alpha,\beta,\nu} e^{i\omega_\nu \epsilon} \left[-i\omega_\nu \delta_{\alpha\beta} + \frac{t_{\alpha\beta} - \delta_{\alpha\beta}\,\mu}{\hbar} \right] \tilde{\phi}^*_{\alpha,\nu}\, \tilde{\phi}_{\beta,\nu}$$

$$= \epsilon \sum_{\alpha,\beta,\nu} e^{i\omega_\nu \epsilon} \left(-G^{-1}_{0,\alpha\beta}(i\omega_\nu) \right) \tilde{\phi}^*_{\alpha,\nu}\, \tilde{\phi}_{\beta,\nu}$$

$$\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - \frac{\mathbf{t} - \mu}{\hbar}$$

Green's function

Our expression for the Green's function was

$$G_{\alpha,\beta}(\tau,\tau') \quad = \quad -\lim_{M\to\infty} \frac{\prod_{k=1}^{M} \prod_{\gamma} \int \; d\phi^{*}_{\gamma,k}\, d\phi_{\gamma,k}\; \phi_{\alpha,k(\tau)} {\phi^{*}}_{\beta,k(\tau')} \; e^{-S(\phi^{*},\phi)}}{\prod_{k=1}^{M} \prod_{\gamma} \int \; d\phi^{*}_{\gamma,k}\, d\phi_{\gamma,k}\; e^{-S(\phi^{*},\phi)}}$$

Not surprisingly the Fourier transform turns out to be

$$G_{\alpha,\beta}(i\omega_{\nu}) \quad = \quad -\frac{\prod_{\mu=-\infty}^{\infty} \; \prod_{\gamma} \int \; d\tilde{\phi}^{*}_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\; \tilde{\phi}_{\alpha,\nu}\; {\tilde{\phi}^{*}}_{\beta,\nu}\; e^{-S(\tilde{\phi}^{*},\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_{\gamma} \; \int \; d\tilde{\phi}^{*}_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\; e^{-S(\tilde{\phi}^{*},\tilde{\phi})}},$$

Our plan

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- We have introduced the Green's function and self-energy
- In 1960 Luttinger and Ward have shown that the grand canonical potential Ω can be expressed as a functional of the Green's function
- We now want to proove this theorem
- Luttinger and Ward employed the technique of Feynman diagrams
- This is questionable for strongly correlated electron systems such as Mott insulators
- We will therefore give a non-perturbative derivation which is due to M. Potthoff and uses functional derivatives instead

Change of perspective

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The Green's function can be represented as a Grassmann functional integral

$$G_{\alpha,\beta}(i\omega_\nu) = -\frac{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\gamma,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

Now we change perspective: all quantities of interest - $\mathbf{G}_0$, $\mathbf{G}$, Σ - all are ultimately sets of complex numbers: $F_{\alpha,\beta}(i\omega_\nu)$, $F \in \{G_0, G, \Sigma\}$

Now take the above as definition of a functional $\mathbf{G}_0 \rightarrow \mathbf{G}$

$$\mathcal{G}[\mathbf{G}_0^{-1}] = -\frac{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}$$

Note: This functional has K_1 - the interaction part of H - as an implicit parameter

Terminology

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In the following we will call a Green's function a 'physical Green's function' if it is the Green's function corresponding to some noninteracting Hamiltonian K_0 (remember that K_1 is fixed - it is a parameter of the functional!)

Similarly for a 'physical self-energy'...

Does that make sense?

- One might wonder if $\mathcal{G}[\mathbf{G}_0^{-1}]$ - and other functionals we define in a moment - is well-defined for any $\mathbf{G}_0$
- The answer is: probably not...
- However $\mathcal{G}[\mathbf{G}_0^{-1}]$ is well defined for physical G_0
- In the following development we will always take functional derivatives of $\mathcal{G}[\mathbf{G}_0^{-1}]$ taken at physical G_0
- This means we need $\mathcal{G}[\mathbf{G}_0^{-1}]$ only for G_0 which are infinitesimally close to physical ones

More functionals

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Recall

$$\mathcal{G}[\mathbf{G}_0^{-1}] = -\frac{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\gamma,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

The next functional

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta} \ln\left(\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right)$$

$\mathbf{G}_0^{-1}(\omega_\nu) = i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar} \Rightarrow \Omega[\mathbf{G}_0^{-1}]$ is the grand canonical potential for $K = K_0 + K_1$

Functional derivative of Ω

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Recall:

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta} \ln \left(\prod_{\mu=-\infty}^{\infty} \prod_{\gamma} \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right)$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\alpha,\beta,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

$$\Rightarrow \frac{\partial S[\tilde{\phi}^*,\tilde{\phi}]}{\partial G^{-1}_{0,\alpha\beta}(i\omega_\nu)} = -e^{i\omega_\nu\epsilon}\, \tilde{\phi}^*_{\alpha,\nu}\, \tilde{\phi}_{\beta,\nu} = e^{i\omega_\nu\epsilon}\, \tilde{\phi}_{\beta,\nu}\, \tilde{\phi}^*_{\alpha,\nu}$$

$$\Rightarrow \beta \frac{\partial \Omega[\mathbf{G}_0^{-1}]}{\partial G^{-1}_{0,\alpha,\beta}(i\omega_\nu)} = e^{i\omega_\nu\epsilon} \frac{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\beta,\nu}\, \tilde{\phi}^*_{\alpha,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$= -e^{i\omega_\nu\epsilon}\, \mathcal{G}[\mathbf{G}_0^{-1}]_{\beta,\alpha}(i\omega_\nu)$$

More functionals...

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For given 'self energy' Σ and given 'Green function' **G** consider

$$\mathbf{D}[\mathbf{G},\Sigma] = \mathcal{G}[\mathbf{G}^{-1}+\Sigma] - \mathbf{G}$$

For physical Green's function and self-energy, **G** and Σ : $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \Sigma$

$$\Rightarrow \mathcal{G}[\mathbf{G}^{-1}+\Sigma] = \mathcal{G}[\mathbf{G}_0^{-1}] = \mathbf{G} \Rightarrow \mathbf{D}[\mathbf{G},\Sigma] = 0$$

Now assume a given 'Green's function' **G** - define a new functional $\mathcal{S}[\mathbf{G}]$ to be the 'self-energy' such that

$$|\mathbf{D}\,[\mathbf{G},\mathcal{S}[\mathbf{G}]]\,| \quad = \quad \sum_{\alpha,\beta}\sum_{\nu} |D_{\alpha,\beta}(i\omega_\nu)|^2 \rightarrow min$$

For physical Green's function and self-energy, **G** and Σ : $\mathbf{D}[\mathbf{G},\Sigma] = 0 \Rightarrow \mathcal{S}[\mathbf{G}] = \Sigma$

Otherwise

$$\mathcal{G}\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right] \quad = \quad \mathbf{G}+\delta\mathbf{G}$$

Summary of functionals

$$S[\tilde{\phi}^*, \tilde{\phi}] = -\sum_{\gamma,\nu} \tilde{\phi}^*_{\gamma,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\gamma,\nu} + K_1[\tilde{\phi}^*, \tilde{\phi}]$$

$$\mathcal{G}[\mathbf{G}_0^{-1}] = -\frac{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}} \rightarrow \mathbf{G}$$

$$\Omega[\mathbf{G}_0^{-1}]_{\alpha,\beta} = -\frac{1}{\beta} \ln\left(\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right) \rightarrow \Omega$$

$$\mathcal{G}\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] = \mathbf{G} + \delta\mathbf{G} \qquad \mathcal{S}[\mathbf{G}] \rightarrow \Sigma, \qquad \delta\mathbf{G} \rightarrow 0$$

Luttinger-Ward functional

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The Luttinger-Ward functional of a Green's function is

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\left[-\ln\ \det \mathbf{G}(i\omega_\lambda) + \text{trace } \mathbf{G}(i\omega_\lambda)\mathcal{S}[\mathbf{G}](i\omega_\lambda)\right]$$

- Physical Green's function: $\mathcal{S}[\mathbf{G}] \to \Sigma$, $\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}] \to \mathbf{G}_0^{-1}$, $\Omega\left[\mathbf{G}_0^{-1}\right] \to \Omega$
- $\ln\ \det \mathbf{G}(i\omega_\nu) = \sum_n \ln(g_n)$ - g_n are the eigenvalues of $\mathbf{G}(i\omega_\nu)$
- In particular, if $\alpha = (\mathbf{k}, \sigma) \Rightarrow \mathbf{G}(i\omega_\nu)$ is diagonal with elements $G(\mathbf{k}, i\omega_\nu)$

$$\ln\ \det \mathbf{G}(i\omega_\nu) = 2\sum_{\mathbf{k}} \ln\ G(\mathbf{k}, i\omega_\nu)$$

- Moreover

$$\text{trace } \mathbf{G}(i\omega_\lambda)\mathcal{S}[\mathbf{G}](i\omega_\lambda) = \sum_{\gamma,\delta} G_{\gamma\delta}(i\omega_\lambda)\mathcal{S}[\mathbf{G}]_{\delta\gamma}(i\omega_\lambda)$$

Functional derivative of Φ

We had ...

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\,\left[\,-\ln\det\mathbf{G}(i\omega_\lambda) + \mathrm{trace}\,\mathbf{G}(i\omega_\lambda)\Sigma[\mathbf{G}](i\omega_\lambda)\,\right]$$

... and want to calculate

$$\beta\,\frac{\partial\Phi}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

To differentiate the first term we recall ...

$$\beta\,\frac{\partial\Omega[\mathbf{G}_0^{-1}]}{\partial G^{-1}_{0,\alpha,\beta}(i\omega_\nu)} \quad = \quad -e^{i\omega_\nu\epsilon}\,\mathcal{G}[\mathbf{G}_0^{-1}]_{\beta,\alpha}(i\omega_\nu)$$

... and use the chain rule (but note that $\mathbf{G}_0^{-1} \to \mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]$)

$$\beta\,\frac{\partial\Omega}{\partial G_{\alpha,\beta}(i\omega_\nu)} \quad = \quad \beta\sum_{\gamma,\delta,\lambda}\frac{\partial\Omega}{\partial G^{-1}_{0,\gamma,\delta}(i\omega_\lambda)}\,\frac{\partial G^{-1}_{0,\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

Functional derivative of Φ

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We had ...

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ [-\ln\det\mathbf{G}(i\omega_\lambda) + \text{trace}\ \mathbf{G}(i\omega_\lambda)\Sigma[\mathbf{G}](i\omega_\lambda)\ ]$$

... and want to calculate

$$\beta\,\frac{\partial\Phi}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

To differentiate the first term we recall ...

$$\beta\,\frac{\partial\Omega[\mathbf{G}_0^{-1}]}{\partial G^{-1}_{0,\alpha,\beta}(i\omega_\nu)} \quad = \quad -e^{i\omega_\nu\epsilon}\ \mathcal{G}[\mathbf{G}_0^{-1}]_{\beta,\alpha}(i\omega_\nu)$$

$$\beta\,\frac{\partial\Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right]}{\partial G_{\alpha,\beta}(i\omega_\nu)} \quad = \quad -\sum_{\lambda}\sum_{\delta,\gamma}\mathcal{G}\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right]_{\delta,\gamma}(i\omega_\lambda)\ \frac{\partial(G^{-1} + \mathcal{S}[\mathbf{G}])_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

Functional derivative of Φ

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$$\beta \frac{\partial \Omega\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right]}{\partial G_{\alpha,\beta}(i\omega_\nu)} = -\sum_\lambda \sum_{\delta,\gamma} \left(G_{\delta,\gamma}+\delta G_{\delta,\gamma}\right)(i\omega_\lambda) \frac{\partial\left(G^{-1}+\mathcal{S}[\mathbf{G}]\right)_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

Next, notice that for each ω_λ

$$\text{trace } \mathbf{G}\mathbf{G}^{-1} = \sum_{\gamma,\delta} G_{\delta,\gamma}(i\omega_\lambda) G^{-1}_{\gamma,\delta}(i\omega_\lambda) = const, \qquad \frac{\partial G_{\delta,\gamma}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} = \delta_{\nu,\lambda}\,\delta_{\alpha,\delta}\,\delta_{\beta,\gamma}$$

$$\Rightarrow \sum_{\gamma,\delta,\lambda}\left(\delta_{\nu,\lambda}\,\delta_{\alpha,\delta}\,\delta_{\beta,\gamma}\,G^{-1}_{\gamma,\delta}(i\omega_\nu) + G_{\delta,\gamma}(i\omega_\lambda)\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}\right) = 0$$

$$\Rightarrow -\sum_{\gamma,\delta} G_{\delta,\gamma}(i\omega_\lambda)\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} = \delta_{\nu,\lambda}\,G^{-1}_{\beta,\alpha}(i\omega_\nu),$$

Functional derivative of Φ

$$\beta \frac{\partial \Omega\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right]}{\partial G_{\alpha,\beta}(i\omega_\nu)} = -\sum_\lambda \sum_{\delta,\gamma} \left(G_{\delta,\gamma}+\delta G_{\delta,\gamma}\right)(i\omega_\lambda) \frac{\partial (G^{-1}+\mathcal{S}[\mathbf{G}])_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

We just found

$$\Rightarrow -\sum_{\gamma,\delta} G_{\delta,\gamma}(i\omega_\lambda) \frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} = \delta_{\nu,\lambda}\, G^{-1}_{\beta,\alpha}(i\omega_\nu)$$

The derivative of the 1st term in the Luttinger-Ward functional is

$$\beta \frac{\partial \Omega\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right]}{\partial G_{\alpha,\beta}(i\omega_\nu)} = G^{-1}_{\beta,\alpha}(i\omega_\nu) - \sum_\lambda \sum_{\delta,\gamma} G_{\delta,\gamma}(i\omega_\lambda) \frac{\partial \mathcal{S}[\mathbf{G}]_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} + 0(\delta G)$$

$$\rightarrow G^{-1}_{\beta,\alpha}(i\omega_\nu) - \sum_\lambda \sum_{\delta,\gamma} G_{\delta,\gamma}(i\omega_\lambda) \frac{\partial \Sigma_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

Functional derivative of Φ

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We had

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ [\,-\ln\det \mathbf{G}(i\omega_\lambda) + \text{trace } \mathbf{G}(i\omega_\lambda)\mathcal{S}[\mathbf{G}](i\omega_\lambda)\ ]$$

To differentiate the second term we use

$$\frac{\partial \ln(\det A)}{\partial A_{\alpha,\beta}} = A^{-1}_{\beta,\alpha}$$

$$\beta\,\frac{\partial}{\partial G_{\alpha,\beta}(i\omega_\nu)}\left(-\frac{1}{\beta}\sum_{\lambda}\ln\det\ \mathbf{G}(i\omega_\lambda)\right) \quad = \quad -G^{-1}_{\beta,\alpha}(i\omega_\nu)$$

Then the last term

$$\mathcal{S}[\mathbf{G}]_{\beta,\alpha}(i\omega_\nu) + \sum_{\lambda}\sum_{\delta,\gamma} G_{\delta,\gamma}(i\omega_\lambda)\frac{\partial \mathcal{S}[\mathbf{G}]_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

Functional derivative of Φ

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Recall

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ [-\ln\det\mathbf{G}(i\omega_\lambda) + \text{trace}\ \mathbf{G}(i\omega_\lambda)\mathcal{S}[\mathbf{G}](i\omega_\lambda)\ ]$$

and

$$\beta\,\frac{\partial\Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right]}{\partial G_{\alpha,\beta}(i\omega_\nu)} = G^{-1}_{\beta,\alpha}(i\omega_\nu) - \sum_{\lambda}\sum_{\delta,\gamma} G_{\delta,\gamma}(i\omega_\lambda)\frac{\partial\mathcal{S}[\mathbf{G}]_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} + 0(\delta G)$$

$$\beta\,\frac{\partial\left(-\frac{1}{\beta}\ \sum_\lambda \ln\det\ \mathbf{G}(i\omega_\lambda)\right)}{\partial G_{\alpha,\beta}(i\omega_\nu)} = -G^{-1}_{\beta,\alpha}(i\omega_\nu)$$

$$\beta\,\frac{\partial\ \text{trace}\ \mathbf{G}(i\omega_\lambda)\mathcal{S}[\mathbf{G}](i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} = \mathcal{S}[\mathbf{G}]_{\beta,\alpha}(i\omega_\nu) + \sum_{\lambda}\sum_{\delta,\gamma} G_{\delta,\gamma}(i\omega_\lambda)\,\frac{\partial\mathcal{S}[\mathbf{G}]_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}$$

Functional derivative

Adding up everything we obtain the final result

$$\beta \frac{\partial \,\Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(i\omega_\nu)} = e^{i\omega_\nu\epsilon}\, \mathcal{S}[\mathbf{G}]_{\beta,\alpha}(i\omega_\nu) + 0(\delta G) \to e^{i\omega_\nu\epsilon}\, \Sigma_{\beta,\alpha}(i\omega_\nu)$$

The derivative of the Luttinger-Ward functional with respect to G is Σ

Recall

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_\lambda e^{i\omega_\lambda\epsilon}\,\left[\,-\ln\det \mathbf{G}(i\omega_\lambda) + \mathrm{trace}\ \mathbf{G}(i\omega_\lambda)\mathcal{S}[\mathbf{G}](i\omega_\lambda)\,\right]$$

For physical G and Σ we obtain the famous expression of Luttinger and Ward for Ω

$$\Omega \quad = \quad -\frac{1}{\beta}\sum_\lambda e^{i\omega_\lambda\epsilon}\,\left(\ln\det\,(\mathbf{G}^{-1}(i\omega_\lambda)) + \mathrm{trace}\ \mathbf{G}(i\omega_\lambda)\Sigma(i\omega_\lambda)\,\right) + \Phi[\mathbf{G}]$$

What we have shown

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- There exists a functional of the Green's function $\Phi[\mathbf{G}]$ such that the Ω can be represented in terms of the Green's function

$$\Omega[\mathbf{G}] \quad = \quad -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\left(\ln\det\left(\mathbf{G}^{-1}(i\omega_\lambda)\right) + \text{trace }\mathbf{G}(i\omega_\lambda)\Sigma(i\omega_\lambda)\right) + \Phi[\mathbf{G}]$$

- $\Phi[\mathbf{G}]$ depends only on the interaction part K_1

Summary of functionals

$$S[\tilde{\phi}^*, \tilde{\phi}] = -\sum_{\gamma,\nu} \tilde{\phi}^*_{\gamma,\nu} \, e^{i\omega_\nu \epsilon} \, G^{-1}_{0,\alpha\beta}(i\omega_\nu) \, \tilde{\phi}_{\gamma,\nu} + K_1[\tilde{\phi}^*, \tilde{\phi}]$$

$$\mathcal{G}[\mathbf{G}_0^{-1}] = -\frac{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu} \, d\tilde{\phi}_{\gamma,\mu} \, \tilde{\phi}_{\alpha,\nu} \, \tilde{\phi}^*_{\beta,\nu} \, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu} \, d\tilde{\phi}_{\gamma,\mu} \, e^{-S(\tilde{\phi}^*,\tilde{\phi})}} \rightarrow \mathbf{G}$$

$$\Omega[\mathbf{G}_0^{-1}]_{\alpha,\beta} = -\frac{1}{\beta} \ln\left(\prod_{\mu=-\infty}^{\infty} \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu} \, d\tilde{\phi}_{\gamma,\mu} \, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right) \rightarrow \Omega$$

$$\mathcal{G}\left[\mathbf{G}^{-1} + \mathcal{S}[\mathbf{G}]\right] = \mathbf{G} + \delta\mathbf{G} \qquad \mathcal{S}[\mathbf{G}] \rightarrow \Sigma, \qquad \delta\mathbf{G} \rightarrow 0$$

What we have shown

- There exists a functional of the Green's function $\Phi[\mathbf{G}]$ such that the Ω can be represented in terms of the Green's function

$$\Omega[\mathbf{G}] = -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\left(\ln\det\left(\mathbf{G}^{-1}(i\omega_\lambda)\right) + \text{trace}\,\mathbf{G}(i\omega_\lambda)\Sigma(i\omega_\lambda)\right) + \Phi[\mathbf{G}]$$

- $\Phi[\mathbf{G}]$ depends only on the interaction part K_1

- The derivative of $\Phi[\mathbf{G}]$ with respect to $\mathcal{G}$ is the self-energy

$$\beta\,\frac{\partial\,\Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(i\omega_\nu)} = e^{i\omega_\nu \epsilon}\,\Sigma_{\beta,\alpha}(i\omega_\nu)$$

- Now we want to change variables and express Ω as a functional of Σ
- This can be done by Legendre transform

Recap Legendre transform

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- Knowing $U(S, V, N)$ contains all thermodynamical information about a system

$$U = U(S, V, N) \qquad \Rightarrow \qquad T(S, V, N) = \frac{\partial U}{\partial S}|_{V,N}$$

- We may change variables by Legendre transform
- Revert $T(S, V, N) \to S(T, V, N)$
- Define $F(T, V, N) = U(\,S(T, V, N), V, N\,) - T\,S(T, V, N)$ - then

$$\frac{\partial F}{\partial T}|_{V,N} = \frac{\partial U}{\partial S}|_{V,N}\,\frac{\partial S}{\partial T}|_{V,N} - S(T, V, N) - T\,\frac{\partial S}{\partial T}|_{V,N} = -S(T, V, N)$$

Since

$$\frac{1}{\beta}\,e^{i\omega_\nu \epsilon}\,\Sigma_{\beta,\alpha}(i\omega_\nu) = \frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(i\omega_\nu)},$$

we can use this formalism to change from $\Phi[G]$ to $F[\Sigma]$

Legendre Transform of Φ

We had

$$\frac{1}{\beta}\, e^{i\omega_\nu \epsilon}\, \Sigma_{\beta,\alpha}(i\omega_\nu) = \frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(i\omega_\nu)},$$

Recall: $\Phi \Leftrightarrow U$, $G_{\alpha,\beta}(i\omega_\lambda) \Leftrightarrow S$ $\frac{1}{\beta}\, e^{i\omega_\nu \epsilon}\, \Sigma_{\beta,\alpha}(i\omega_\lambda) \Leftrightarrow T$

$\Rightarrow F = U - S\, T$ becomes

$$F[\Sigma] = \Phi\,[\mathbf{G}[\Sigma]] - \frac{1}{\beta} \sum_{\lambda} \sum_{\gamma,\delta} G[\Sigma]_{\delta,\gamma}(i\omega_\lambda)\; e^{i\omega_\lambda \epsilon}\, \Sigma_{\gamma,\delta}(i\omega_\lambda)$$

$$= \Phi\,[\mathbf{G}[\Sigma]] - \frac{1}{\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon}\, \text{trace}\; \mathbf{G}[\Sigma](i\omega_\lambda)\Sigma(i\omega_\lambda)$$

Legendre Transform of Φ

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We had

$$\Omega[G] = -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\left(\ln\det\left(\mathbf{G}^{-1}(i\omega_\lambda)\right) + \text{trace } G(i\omega_\lambda)\,\Sigma(i\omega_\lambda)\right) + \Phi[\mathbf{G}]$$

and

$$F[\Sigma] = \Phi\left[\mathbf{G}[\Sigma]\right] - \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\,\text{trace } \mathbf{G}[\Sigma](i\omega_\lambda)\Sigma(i\omega_\lambda)$$

Combining this we find

$$\begin{aligned}\Omega[\Sigma] &= -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\,\ln\det\left(\mathbf{G}^{-1}(i\omega_\lambda)\right) + F[\Sigma] \\ &= -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\,\ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma]\end{aligned}$$

Stationarity of Ω

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$$\Omega[\Sigma] \quad = \quad -\frac{1}{\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \; \ln\det \left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda) \right) + F[\Sigma]$$

Since $F[\Sigma]$ is the Legendre transform of $\Phi[G]$ we know that

$$\beta \, \frac{\partial F[\Sigma]}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad -e^{i\omega_\nu \epsilon} \; G_{\beta,\alpha}(i\omega_\nu)$$

This is the equivalent of $\frac{\partial F}{\partial T} = -S$

Therefore

$$\beta \, \frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad e^{i\omega_\nu \epsilon} \; G_{\beta,\alpha}(i\omega_\nu) - e^{i\omega_\nu \epsilon} \; G_{\beta,\alpha}(i\omega_\nu) = 0$$

We have represented Ω as a functional of Σ

This functional is stationary at the exact Σ

Summary

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- There exists a functional of the self energy $F[\Sigma]$ such that Ω is

$$\Omega[\Sigma] \quad = \quad -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ \ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma].$$

- $F[\Sigma]$ depends only on the intraction part K_1
- The Grand canonical potential is stationary under variations of Σ

$$\frac{\partial\Omega}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad 0$$

- The Green's function is the variation of $F[\Sigma]$

$$\beta\,\frac{\partial F[\Sigma]}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad -e^{i\omega_\nu\epsilon}\, G_{\beta,\alpha}(i\omega_\nu),$$

Variational principle emerging

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- We have seen that Ω can be expressed as a functional of the self energy ....

$$\Omega[\Sigma] \quad = \quad -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon} \ \ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma]$$

- ... which is stationary at the exact self-energy

$$\frac{\partial\Omega}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad 0$$

We therefore might choose a 'trial self-energy' of the form

$$\Sigma(i\omega_\nu) \quad = \quad const + \int_{-\infty}^{\infty} d\omega \ \frac{\sigma(\omega)}{\omega - i\omega_\nu}.$$

and derive the Euler-Lagrange equation for $\sigma(\omega)$!

Dynamical mean-field theory

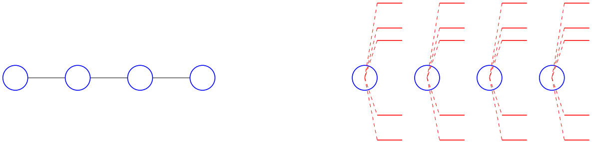
Consider the Hubbard model with N sites and pbc

$$H = \sum_{i,j}\sum_{\sigma} t_{i,j}\, c^{\dagger}_{i,\sigma} c_{i,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow}$$

In addition consider the ‘reference system’

$$\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$$

$$\tilde{H}_i = \sum_{\nu} \epsilon_{\nu}\, l^{\dagger}_{i,\nu,\sigma}\, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_{\nu}\, l^{\dagger}_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U\, n_{i,\uparrow} n_{i\downarrow}$$



Dynamical mean-field theory

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Consider the Hubbard model with N sites and pbc

$$H = \sum_{i,j} \sum_{\sigma} t_{i,j}\, c^{\dagger}_{i,\sigma} c_{i,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow}$$

In addition consider the ‘reference system’

$$\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$$

$$\tilde{H}_i = \sum_{\nu} \epsilon_{\nu}\, l^{\dagger}_{i,\nu,\sigma}\, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_{\nu}\, l^{\dagger}_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U\, n_{i,\uparrow} n_{i\downarrow}$$

The crucial point: Both models have the same interaction term

$$K_1 = U \sum_{i} n_{i,\uparrow} n_{i\downarrow}$$

Dynamical mean-field theory

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- Hubbard model and reference system have the same $F[\Sigma]$
- The 'ligands' $l^{\dagger}_{i,\nu,\sigma}$ are uncorrelated - only $\tilde{\Sigma}_{c,c}(i\omega_\lambda)$ is different from zero

$$\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$$

$$\tilde{H}_i = \sum_{\nu} \epsilon_\nu \, l^{\dagger}_{i,\nu,\sigma} \, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_\nu \, l^{\dagger}_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U \, n_{i,\uparrow} n_{i\downarrow}$$

- Ω is stationary under variations of the self-energy - we restrict the 'domain of self-energies' to those of the reference system $\tilde{\Sigma}_{c,c}(i\omega_\lambda)$

$$\frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = 0 \quad \Rightarrow \quad \frac{\partial \Omega}{\partial t} = 0$$

with $t \in \{\epsilon_\nu, V_\nu\}$

Dynamical mean-field theory

Recall:

$$\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$$

$$\tilde{H}_i = \sum_{\nu} \epsilon_\nu \, l^\dagger_{i,\nu,\sigma} \, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_\nu \, l^\dagger_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U \, n_{i,\uparrow} n_{i\downarrow}$$

We compute the derivative of $F[\tilde{\Sigma}]$ with respect to a parameter $t \in \{\epsilon_\nu, V_\nu\}$

$$\frac{\partial F[\tilde{\Sigma}]}{\partial t} = \sum_{\alpha,\beta} \sum_{\lambda} \frac{\partial F[\tilde{\Sigma}]}{\partial \tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)} \frac{\partial \tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}{\partial t}$$

$$= -\frac{1}{\beta} \sum_{\alpha,\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \, \tilde{G}_{\beta,\alpha}(i\omega_\lambda) \frac{\partial \tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}{\partial t}$$

$$= -\frac{2N}{\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \, \tilde{G}_{c,c}(i\omega_\lambda) \frac{\partial \tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t}$$

Dynamical mean-field theory

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We apply our general formula ...

$$\Omega[\Sigma] \quad = \quad -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda\epsilon} \; \ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma].$$

... to the Hubbard model

$$\Omega_{latt} \quad = \quad -\frac{2}{\beta}\sum_{\mathbf{k}}\sum_{\lambda} e^{i\omega_\lambda\epsilon} \; \ln\left[i\omega_\lambda - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \tilde{\Sigma}_{c,c}(i\omega_\lambda)\right] + F[\tilde{\Sigma}]$$

We recall

$$\frac{\partial F[\tilde{\Sigma}]}{\partial t} \quad = \quad -\frac{2N}{\beta}\sum_{\lambda} e^{i\omega_\lambda\epsilon} \; \tilde{G}_{c,c}(i\omega_\lambda) \; \frac{\partial\tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t}$$

$$\Rightarrow \frac{\partial\Omega_{latt}}{\partial t} \quad = \quad \frac{2}{\beta}\sum_{\lambda} e^{i\omega_\lambda\epsilon} \left[\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) - N\tilde{G}_{c,c}(i\omega_\lambda)\right] \frac{\partial\tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t} = 0$$

Dynamical mean-field theory

We found that for any $t \in \{\epsilon_\nu, V_\nu\}$

$$\frac{\partial \Omega_{latt}}{\partial t} = \frac{2}{\beta} \sum_\lambda e^{i\omega_\lambda \epsilon} \left[\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) - N\, \tilde{G}_{c,c}(i\omega_\lambda) \right] \frac{\partial \tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t} = 0$$

The simplest way to solve this is to set for each ω_λ

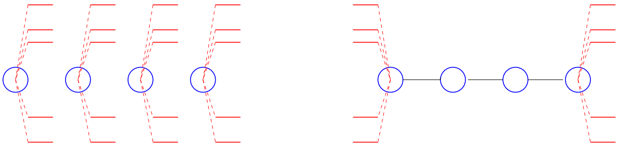
$$\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) - N\, \tilde{G}_{c,c}(i\omega_\lambda) = 0$$

$$\Rightarrow \tilde{G}_{c,c}(i\omega_\lambda) = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{i\omega_\lambda - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \tilde{\Sigma}_{c,c}(i\omega_\lambda)}$$

This is precisely the self-consistency equation for Dynamical Mean-Field Theory!

Generalizations

In the same way one can derive cluster generalizations of dynamical mean-field theory



Another way is to numerically evaluate the Luttinger-Ward functional in the reference system - this is the Variational Cluster Approximation

And there is probably more to be discovered...for example even an approximate form of $F[\Sigma]$

Summary

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- We have seen that the grand canonical potential of an interacting electron system can be expressed as a functional of its self-energy: $\Omega[\Sigma]$
- This functional is stationary at the exact self-energy
- Unfortunately this involves (the Legendre transform of) the Luttinger-Ward functional for which we do not have any explicit expression
- This problem can be circumvented by combination with numerical methods - a.g. in dynamical mean-field theory or cluster generalizations